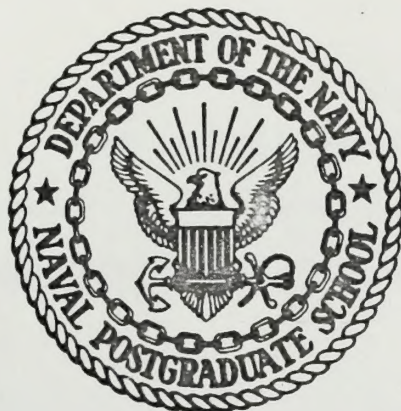


CALCULATION OF ELECTRON SCATTERING CROSS
SECTIONS FOR CARBON-TWELVE AND
LITHIUM-SIX USING PHASE SHIFT ANALYSIS

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THESIS

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Sections for Carbon-Twelve and Lithium-Six Using
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June 1970

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Sections for Carbon-Twelve and Lithium-Six Using
Phase Shift Analysis

by

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ABSTRACT

A phase shift analysis is used to obtain scattering cross sections for incident electrons on Carbon-12 and Lithium-6. Results are given for incident electron energies of 10-100 Mev and for scattering angles of 45, 90 and 135 degrees. A gaussian p-shell charge distribution is used for Carbon-12, and an empirical charge distribution developed by L. R. Suelzle is used for Lithium-6. A comparison is also made between the phase-shift results and results obtained using the Born approximation.

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I. INTRODUCTION

Many experiments on the elastic scattering of high energy electrons from nuclei have been conducted in an effort to understand the structure of the nuclei. That the nuclear charge distribution has finite extension has been clearly exhibited [1, 2]. The exact form of this charge distribution is not known, although many theoretical and empirical models have been proposed. From experiments, it has been tentatively concluded that this charge distribution peaks at the center of the nucleus, and tapers off at the edge. This conclusion is reached using the Born approximation, which is most accurate for light nuclei.

The fact that the Born approximation is not accurate for heavy elements led Yennie, Ravenhall and Wilson [3] to carry out a phase shift analysis of the scattering process. This analysis neglected the mass of the electron, which is a good approximation for very high energy electrons. Another phase shift analysis by Rawitscher [4] did not make this approximation and is therefore apparently a more accurate calculation. It is the phase shift analysis by Rawitscher which forms the basis for this work.

The model used for this "exact" phase shift analysis is the Dirac equation for an electron in the electrostatic potential of a static, spherically symmetric charge distribution. The interaction of the electron with nuclear magnetic or electric quadrupole moments, and possible nuclear excitation is neglected in this analysis. Calculations done by Schiff [6] using the first Born approximation suggest that the magnetic quadrupole moment interaction is negligible at high energies, and reference [3] suggests that the electric quadrupole moment and nuclear excitation interactions are negligible except for a few particular elements at large angles.

The electron scattering experiments conducted at this facility are of relatively low energy, 20 - 100 Mev, when compared to energies available at other linear accelerators. For this given range of energy, and for light nuclei, the Born approximation should provide a good method for calculation of scattering cross sections. A comparison of results, using the Born approximation and phase shift analysis, for light nuclei is given in Section III. The computer program which accomplishes the desired calculations is contained herein following Appendix A. All calculations were done on the IBM 360 computer available at this facility. The program is written in FORTRAN and comments are located in various sections to aid in understanding.

II. METHOD OF CALCULATION

The well-known Dirac equation forms the basis of the calculations, and it is from it that the scattered wave function is obtained by the method of partial wave expansion [5]. As was stated earlier, the potential acting on the electron is assumed to be entirely the result of a static Coulomb interaction arising from a charge distribution $\rho(r)$.

The program has built into it many different forms for $\rho(r)$. Those used for calculation of results in Section III are shown below:

(1) gaussian p-shell:

$$\rho(r) = \rho_0 \left[1 + \alpha \left(\frac{r}{a} \right)^2 \right] \exp \left[- \left(\frac{r}{a} \right)^2 \right]$$

(2) Li^6 :

$$\rho(r) = \frac{1}{8\pi^{3/2}} \left[\frac{1}{a^3} \exp \left(- \frac{r^2}{4a^2} \right) - \frac{c^2 (6b^2 - r^2)}{4b^7} \exp \left(- \frac{r^2}{4b^2} \right) \right]$$

The second one above, (2), is an empirical form obtained from the work of Suelzle, Yearian, and Crannell [7]. In the above forms, r is the radial distance from the center of the nucleus. The potential inside the charge distribution may be calculated using the expression:

$$-V(r) = \frac{4\pi \left(\frac{Ze^2}{\hbar c} \right)}{r} \int_0^r e(r^1) r^{1^2} dr^1 + 4\pi \left(\frac{Ze^2}{\hbar c} \right) \int_r^\infty e(r^1) r^1 dr^1$$

while the potential outside the nucleus is of the form

$$V(r) = - \frac{Ze^2}{\hbar cr}$$

The scattering wave function, in the partial wave analysis, is regarded as a series of eigenfunctions of the operator k , which is related to the angular momentum for Dirac Particles. (8). The radial wave functions $F_k(x)$ and $G_k(x)$ obey the radial equations:

$$\left(\frac{d}{dx} - \frac{k}{x} \right) g_k + (1 - v_1) f_k = 0$$

$$\left(\frac{d}{dx} + \frac{k}{x}\right)f_k - (1 - V_2) g_k = 0$$

where

$$G_k = r^{-1} (E + 1)^{\frac{1}{2}} g_k, \quad F_k = r^{-1} (E - 1)^{\frac{1}{2}} f_k$$

See Appendix A for explanation of symbols and further details. The asymptotic behavior of the F's and G's determines the phase shifts η_k from which $f(\theta)$ and $g(\theta)$ and finally the cross section is calculated

The integration of the above radial equations must be done numerically. The method used is outlined in reference [3]. It is essentially a step-by-step procedure based on derivatives rather than on differences, following formulas given in reference [9].

Starting with a regular solution obtained by a power series expansion about the origin [10], the radial equations are integrated from $x = 1/1024$ to a fitting radius x_0 . From the Appendix, $x = r_0 \kappa$, where $\kappa = mc p / \hbar$ and $p = \text{momentum}/mc$. At x_0 , the $f_k(x_0)$ and $g_k(x_0)$ are fitted to two pairs of linearly independent Coulomb functions:

$$\begin{aligned} g_k(x_0) &= C_k g_k^R(x_0) + D_k g_k^I(x_0) \\ f_k(x_0) &= C_k f_k^R(x_0) + D_k f_k^I(x_0) \end{aligned}$$

I, R refer to Coulomb functions which are regular (R) or irregular (I), at the origin

The major difference in the phase-shift analysis used here and the one developed by Yennie et al, shows up in the calculation of the phase shift η_k . Due to the inclusion of the rest mass of the electron in the total energy, the value of the phase shift for $+k$ values is not equal to the phase shift of $-k$, and must be calculated separately.

The scattering amplitudes $f(\theta)$ and $g(\theta)$ are obtained from the phase shifts and Legendre polynomials by a summation procedure found satisfactory

in reference [3]. A change in the normal summation procedure was made to improve the convergence of the Coulomb scattering amplitude series.

The new summation procedure, that of reference [3], is designed to transform $f(\theta)$ to make it less singular at small values of θ . This is accomplished by multiplying $f(\theta)$ by a function which vanishes at $\theta = 0$ and then expanding the new function in a series of Legendre polynomials. First, $f(\theta)$ is represented by

$$2ikf = \sum_k c_k P_k(\cos \theta)$$

The m th reduced series is defined by:

$$(1 - \cos \theta)^m 2ikf = \sum_k c_k^{(m)} P_k(\cos \theta)$$

A similar set of expressions exists for $g(\theta)$ and can be found in Appendix A.

A value of $m = 3$ was used in reference [3] and reference [4]. In this work, a value of $m = 4$ was used in order to compare with referenced results to insure the rapid convergence of the series, and to note the effect of a change in m .

The program was checked out by comparison with published results. The phase shifts and coefficients of the Legendre series for the Coulomb scattering amplitude (Table I and II respectively of Ref. [3]) were reproduced with good accuracy. Also, cross sections for scattering from Carbon-12 at an incident electron energy of 60 Mev, obtained from Yale University, were matched with good agreement. The Yale results were obtained using the same program with $m = 3$.

All of the calculations are done in the center-of-mass system. The laboratory input parameters are converted to this system by the formulas generated using the well-known transformation laws provided by the special theory of relativity. The equations used are contained in reference [11].

III. RESULTS

The results for various conditions in the electron-nucleus scattering process are contained in Tables I - VI. All cross sections are given in f^2 . Tables I - IV contain the phase shift cross section and a quantity called "Phase Shift Formfactor Squared", which is the ratio of the phase shift cross section to the Mott point nucleus cross section. Tables V and VI contain the phase shift cross section, the "Phase Shift Formfactor Squared", and a quantity called "Born Formfactor Squared". The "Born Formfactor Squared" is the ratio of the Born approximation cross section to the Mott cross section. The incident electron energies used are 10 - 100 MeV for Tables I - IV and 10 - 150 MeV for Tables V and VI. All results are given for scattered electron angles of 45° , 90° , and 135° .

The Born form factor is a derived quantity and is related to the Fourier transform of the charge distribution. A plot of the Born form factor versus the transferred momentum from the electron to the nucleus yields the radius of the nucleus by the slope of the plot near the origin. The "Phase Shift Formfactor" does not have such a simple interpretation.

The results in Table I are for the Carbon-12 nucleus. The charge distribution used is the gaussian p-shell model, mentioned earlier in Section II. The parameter values used are $a = 1.648f$ and $\alpha = 1.056$.

The results in Table II are for the same conditions as Table I with the exception that the value of the parameter, a , was changed to give a 10% increase in the rms radius of Carbon-12. This new value is $a = 1.813f$. The value of α was not changed.

From the results, this change in the value of the parameter, a , produced a percentage change in the phase shift cross section ranging from 0.06% at 10 MeV to 6% at 100 MeV, for a scattering angle of 45° .

Table III contains results for scattering from the Lithium-6 nucleus. The charge distribution used is the empirical form developed by Suelzle, and was also mentioned earlier in Section II. The parametric values used were $a^2 = 0.87f$, $b^2 = 1.70f$, and $c^2 = 0.205f$.

The results of Table IV are for the same conditions as Table III with the exception that the value of the parameter, a , was changed to give a 10% increase in the rms radius of Lithium-6. The new value is $a^2 = 1.195f^2$. Approximately the same percentage change in the phase shift cross section was observed here as for Carbon-12.

Tables V and VI contain results for the same conditions as Tables I and III, with the addition of the quantity Born Formfactor Squared. The expressions used for the calculations of the Born Formfactor are:

For Carbon-12, from reference [13]

$$F(q^2) = [1 - \alpha a^2 q^2 / 2(2 + 3\alpha)] \exp(-\frac{1}{4}q^2 a^2)$$

where a and α are the same parameters used in Table I and q is the momentum transfer.

For Lithium-6, from reference [7]

$$F(q^2) = \exp(-a^2 q^2) - c^2 q^2 \exp(-b^2 q^2)$$

where a^2 , b^2 , and c^2 are the same parameters used in Table III.

While the same parameters for the given charge distribution were used in Tables V and VI, as compared to I and II, there was a change made in the value of the fitting radius used for the two cases. In the numerical integration routine used, integration is from the origin out to x_0 , where, as was mentioned earlier, $x_0 = r_0 \kappa$. Since κ is a function of the momentum, and hence the incident energy of the electron, an increase in the energy will cause an increase in the value of x_0 . The step size, or spacing between points where step-by-step integration is done, is a fixed parameter. Thus, for given storage space in the computer, there exists an energy at

which all storage will be utilized prior to reaching x_0 in the integration process. For high energies, this problem can be alleviated by lowering the value of r_0 , the fitting radius in fermi's.

To circumvent this storage problem inherent in using energies above 100 MeV, a fitting radius value of 8.0f was used for all calculations in Tables V and VI, compared to a value of 10.0 used for calculations in Tables I, II, III, and IV. The effect of this change in fitting radius value can be seen by comparison of the phase shift cross section results between Tables I and V, or between Tables III and VI. Also shown in Figure 1, is a plot of the difference between the "Phase Shift Formfactor Squared" and the "Born Formfactor Squared", labeled as $F_p^2 - F_b^2$, as a function of incident electron energy.

IV CONCLUSIONS

The "exact" phase shift analysis provides a means for comparison of theoretical results with experimental data. To uniquely find a charge distribution which fits all experimental data requires more calculations than are given here. The value of the phase-shift analysis lies in its applicability to any scattering situation, being restricted only by the numerical methods used. Many more charge distributions could, and should, be used to compare results with those given here.

A comparison of the results obtained using the phase shift analysis and the Born approximation can be made from the values of "Phase Shift Formfactor Squared" and "Born Formfactor Squared", since both of the quantities represent the respective cross-sections divided by the Mott cross-section. Agreement between these results is good at small angle scattering for all energies considered. Deviation between the two occurs for large angle scattering at energies above 150 Mev. While the exact cause for this deviation is not known, it is believed to be due to particular numerical techniques used.

TABLE I

Carbon-12

Incident electron energy = E

Angle in degrees	Phase Shift Cross Section, f^2	Phase Shift Formfactor Squared
E = 10 MeV		
45	7.6990	1.0311
90	0.39459	1.0500
135	0.040232	1.0526
E = 20 MeV		
45	1.9077	1.0264
90	0.094976	1.0176
135	0.0093839	0.99842
E = 30 MeV		
45	0.83991	1.0181
90	0.040004	0.96652
135	0.0037821	0.90963
E = 40 MeV		
45	0.46169	0.99538
90	0.020885	0.89814
135	0.0018695	0.80133
E = 50 MeV		
45	0.28845	0.97210
90	0.012170	0.81867
135	0.0010046	0.67421
E = 60 MeV		
45	0.19151	0.92960
90	0.0074793	0.72516
135	0.00056986	0.55164
E = 70 MeV		
45	0.13570	0.89680
90	0.0047274	0.62444
135	0.00032788	0.43274
E = 80 MeV		
45	0.099369	0.85799
90	0.0030472	0.52621
135	0.00018908	0.32648
E = 90 MeV		
45	0.074077	0.80976
90	0.0019975	0.43698
135	0.00011137	0.24378

TABLE I (continued)

Carbon-12

Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section, f^2	Phase Shift Formfactor Squared
E = 100 MeV		
45	0.056797	0.76673
90	0.0013337	0.36055
135	0.000067867	0.18369

TABLE II

Carbon-12

Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 10 MeV		
45	7.6939	1.0304
90	0.39370	1.0476
135	0.040076	1.0485
E = 20 MeV		
45	1.9026	1.0237
90	0.094112	1.0083
135	0.0092373	0.98283
E = 30 MeV		
45	0.83500	1.0121
90	0.039188	0.94680
135	0.0036472	0.87718
E = 40 MeV		
45	0.45704	0.98535
90	0.020134	0.86588
135	0.0017494	0.74985
E = 50 MeV		
45	0.28373	0.95619
90	0.011522	0.77506
135	0.00091793	0.61602
E = 60 MeV		
45	0.18706	0.90802
90	0.0068797	0.66879
135	0.00049508	0.47925
E = 70 MeV		
45	0.13150	0.86904
90	0.0042364	0.55958
135	0.00027068	0.35724
E = 80 MeV		
45	0.095369	0.82345
90	0.0026531	0.45503
135	0.00014646	0.25289
E = 90 MeV		
45	0.070329	0.76879
90	0.0016602	0.36318
135	0.000080749	0.17675

TABLE II (continued)

Carbon-12

Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 100 MeV		
45	0.053271	0.71914
90	0.0010604	0.28665
135	0.000045816	0.12401

TABLE III

Lithium-6

Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 10MeV		
45	1.9056	1.0206
90	0.095426	1.0161
135	0.0097114	1.0172
E = 20 MeV		
45	0.46574	1.0027
90	0.022975	0.98622
135	0.0022619	0.96539
E = 30 MeV		
45	0.20439	0.99158
90	0.0086254	0.93253
135	0.00090224	0.87180
E = 40 MeV		
45	0.10904	0.94119
90	0.0050287	0.86796
135	0.00044621	0.76960
E = 50 MeV		
45	0.070536	0.95198
90	0.0029227	0.78985
135	0.00023978	0.64855
E = 60 MeV		
45	0.046945	0.91286
90	0.0017908	0.69819
135	0.00012923	0.50501
E = 70 MeV		
45	0.033412	0.88483
90	0.0011178	0.59428
135	0.000076337	0.40736
E = 80 MeV		
45	0.024142	0.83549
90	0.00071629	0.49826
135	0.000044432	0.31067
E = 90 MeV		
45	0.018222	0.79849
90	0.00047169	0.41600
135	0.000028127	0.24969

TABLE III (continued)

Lithium-6

Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 100 MeV		
45	0.013743	0.74393
90	0.00031767	0.34651
135	0.000018638	0.20491

TABLE IV

Lithium-6

Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 10 MeV		
45	1.9037	1.0196
90	0.095103	1.0126
135	0.0096554	1.0114
E = 20 MeV		
45	0.46391	0.99872
90	0.022665	0.97290
135	0.0022094	0.94300
E = 30 MeV		
45	0.20261	0.98296
90	0.0093330	0.90420
135	0.00085429	0.82547
E = 40 MeV		
45	0.10728	0.92593
90	0.0047658	0.82259
135	0.00040810	0.70388
E = 50 MeV		
45	0.068858	0.92933
90	0.0026828	0.72501
135	0.0020581	0.55667
E = 60 MeV		
45	0.045327	0.88140
90	0.0015750	0.61405
135	0.00010631	0.141544
E = 70 MeV		
45	0.031853	0.84354
90	0.00094298	0.50132
135	0.000056556	0.30180
E = 80 MeV		
45	0.022675	0.78470
90	0.00057131	0.39741
135	0.000029902	0.20907
E = 90 MeV		
45	0.016833	0.73763
90	0.00035251	0.31089
135	0.000017085	0.15167
E = 100 MeV		
45	0.012450	0.67394
90	0.00022082	0.24087
135	0.000010435	0.11473

TABLE V

Carbon-12

Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared	Born Formfactor Squared
E = 10 MeV			
45	7.6990	1.0311	0.99713
90	0.39459	1.0500	0.99023
135	0.040231	1.0525	0.98344
E = 20 MeV			
45	1.9073	1.0262	0.98854
90	0.094906	1.0168	0.96153
135	0.0093720	0.99715	0.93527
E = 30 MeV			
45	0.83967	1.83967	0.97444
90	0.039964	0.96554	0.91544
135	0.0037755	0.90803	0.86007
E = 40 MeV			
45	0.46130	0.99455	0.95501
90	0.020922	0.89544	0.85460
135	0.0018594	0.79700	0.76472
E = 50 MeV			
45	0.28774	0.96971	0.93958
90	0.012161	0.81806	0.78205
135	0.0010189	0.68378	0.65708
E = 60 MeV			
45	0.19110	0.92761	0.90156
90	0.007195	0.72906	0.70152
135	0.00057588	0.55747	0.54537
E = 70 MeV			
45	0.13546	0.89522	0.86835
90	0.0047951	0.63338	0.61663
135	0.00032714	0.43176	0.43680
E = 80 MeV			
45	0.099336	0.85770	0.83149
90	0.0031078	0.53666	0.53104
135	0.00018924	0.32675	0.33726
E = 90 MeV			
45	0.074312	0.81233	0.79159
90	0.0020247	0.44292	0.44767
135	0.00010737	0.23501	0.25062

TABLE V (continued)

Carbon-12

Incident Electron Energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared	Born Formfactor Squared
E = 100 MeV			
45	0.057197	0.77214	0.74914
90	0.0013247	0.35812	0.36938
135	0.000060509	0.16378	0.17892
E = 150 MeV			
45	0.017031	0.51795	0.51978
90	0.00015640	0.095549	0.09931
135	0.0000022275	0.013672	0.01574

TABLE VI

Lithium-6

Incident Electron Energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared	Born Formfactor Squared
E = 10 MeV			
45	1.9056	1.0206	0.99679
90	0.095424	1.0160	0.98908
135	0.0097111	1.0172	0.98146
E = 20 MeV			
45	0.46560	1.0024	0.98719
90	0.022952	0.98521	0.95712
135	0.0022579	0.96370	0.92817
E = 30 MeV			
45	0.20424	0.99083	0.97138
90	0.0095998	0.93005	0.90645
135	0.00089803	0.86773	0.84682
E = 40 MeV			
45	0.10880	0.93908	0.94985
90	0.0050181	0.86614	0.84075
135	0.00044916	0.77469	0.74646
E = 50 MeV			
45	0.070242	0.04801	0.92291
90	0.0029116	0.78685	0.76421
135	0.00024328	0.65802	0.63964
E = 60 MeV			
45	0.046778	0.90962	0.89118
90	0.0017999	0.70170	0.68125
135	0.00013537	0.52899	0.52724
E = 70 MeV			
45	0.03328	0.88262	0.85527
90	0.0011456	0.60903	0.59617
135	0.000078033	0.41641	0.42424
E = 80 MeV			
45	0.024143	0.83550	0.81587
90	0.00074133	0.51568	0.51267
135	0.000044886	0.31384	0.33253
E = 90 MeV			
45	0.018326	0.80308	0.77375
90	0.00048518	0.42790	0.43357
135	0.000026574	0.23590	0.25431

TABLE VI (continued)

Lithium-6

Incident Electron Energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared	Born Formfactor Squared
E = 100 MeV			
45	0.013904	0.75263	0.72951
90	0.00031586	0.34454	0.36096
135	0.000015852	0.17429	0.19003
E = 150 MeV			
45	0.0039987	0.48824	0.50086
90	0.000049157	0.12171	0.11665
135	0.0000012616	0.031705	0.031708

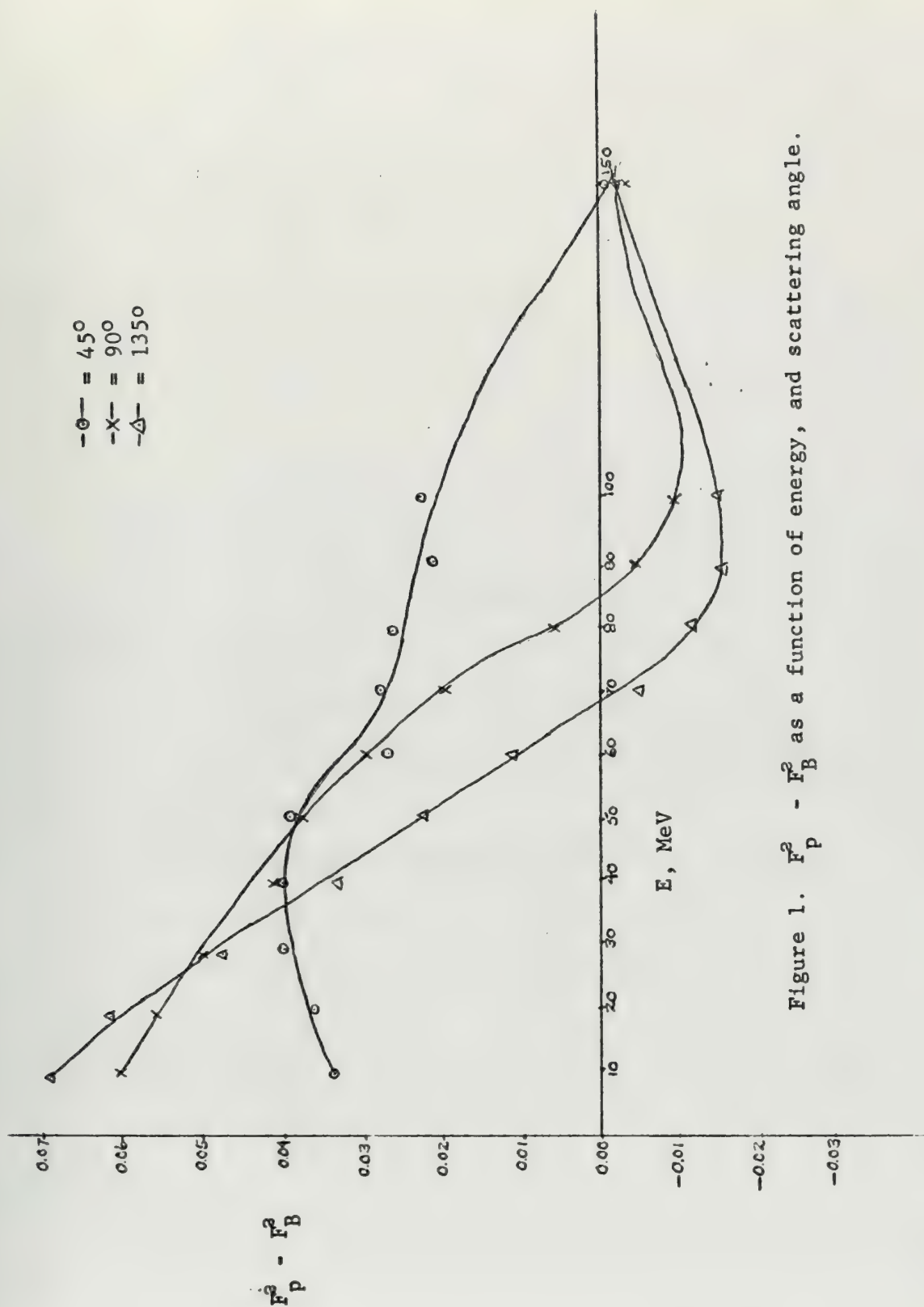


Figure 1. $F_p^2 - F_B^2$ as a function of energy, and scattering angle.

APPENDIX A

The notations and method of calculation used are those of Rawitscher [4], and are shown here for convenience:

The following notation is used,

$$E = \text{total energy}/mc^2$$

$$p = \text{momentum}/mc$$

$$\alpha = Ze^2/\hbar c$$

$$\beta = v/c = p/E$$

$$\gamma = \alpha/\beta$$

$$\gamma' = (1 - \beta^2)^{\frac{1}{2}}$$

$$s_k = + (k^2 - \alpha^2)^{\frac{1}{2}} \text{ for regular solutions, denoted by superscript R,}$$

$$s_k = - (k^2 - \alpha^2)^{\frac{1}{2}} \text{ for irregular solutions, denoted by superscript I,}$$

$$\kappa = mcp/\hbar$$

$$r = \text{radial distance from center of nucleus}$$

$$x = r\kappa, x_0 = r_0\kappa, \text{ where } r_0 \text{ is the matching of fitting-on radius}$$

$$mc^2 = 0.511 \text{ MeV}$$

$$k = \text{angular momentum quantum number } \pm 1, \pm 2, \dots$$

The radial wave functions $F_k(x)$ and $G_k(x)$, defined by

$$G_k = r^{-1}(E + 1)^{\frac{1}{2}}g_k, \quad F_k = r^{-1}(E - 1)^{\frac{1}{2}}f_k \quad (1a)$$

obey the radial equations

$$(d/dx - k/x)g_k + (1 - v_1)f_k = 0 \quad (2a)$$

$$(d/dx + k/x)f_k - (1 - v_2)g_k = 0$$

where

$$v_1 = \Phi(E - 1)/p^2, \quad v_2 = \Phi(E + 1)/p^2, \quad (3a)$$

and where Φ is the Coulomb potential energy in units of mc^2 . For the example of a point nucleus, $\Phi/p = -\alpha/x$.

The phase shifts η_k are defined in the usual manner [5] by the

asymptotic form of the radial wave functions of Eq. (1a):

$$\begin{aligned} G_k &\approx r^{-1} \sin [x - (k - 1) \pi/2 + \eta_k], \quad k > 0 \\ &\approx r^{-1} \sin [x - |k| \pi/2 + \eta_k], \quad k < 0 \end{aligned} \quad (4a)$$

The value of η_k is obtained in terms of the regular and irregular Coulomb phase shifts η_k^R , η_k^I and the matching coefficients $(D/C)_k$ from

$$\tan \eta_k = \frac{\sin \eta_k^R + (D/C)_k \sin \eta_k^I}{\cos \eta_k^R + (D/C)_k \cos \eta_k^I} \quad (5a)$$

The Coulomb phase shifts are given by

$$\eta_k^{R, I} = (X + Y)_k^{R, I} \quad (6a)$$

$$X_k = (k - 1 - s_k) \pi/2 - \arg \Gamma(s_k + 1 + i\gamma), \quad k > 0 \quad (7a)$$

$$X_k = X_{|k|} + \pi/2 \quad k < 0$$

For the sake of clarity the superscripts R and I have been omitted in the above equation. The value of the argument of Γ is calculated by means of Stirling's approximation [12]. The value of Y is given in expression below, valid for both signs of k:

$$\begin{aligned} \sin Y_k &= -k[k(k + s_k) + \gamma'(\gamma' - \gamma)]^{\frac{1}{2}} / (|k| |k - i\gamma'| 2^{\frac{1}{2}}) \\ \cos Y_k &= [k(k - s_k) + \gamma'(\gamma' + \gamma)]^{\frac{1}{2}} / (|k - i\gamma'| 2^{\frac{1}{2}}) \end{aligned} \quad (8a)$$

The matching coefficients $(D/C)_k$ are obtained in terms of the radial wave functions evaluated at x_0 :

$$(D/C)_k = \left[\frac{g'^R - f'^R(g/f)}{(g/f)f'^I - g'^I} \right]_k (N^R/N^I)_k x_0^{2|s_k|} \quad (9a)$$

Here g and f are the solutions of Eqs. (2a) and the primed quantities are related to the point Coulomb radial waves $G^{R, I}$, $F^{R, I}$ by means of

$$\begin{aligned} G_k^{R, I} &= r^{-1} N_k^{R, I} x_0^{s_k} g_k^{R, I} \\ F_k^{R, I} &= r^{-1} [(E - 1)/(E + 1)]^{\frac{1}{2}} N_k^{R, I} x_0^{s_k} f_k^{R, I} \end{aligned} \quad (10a)$$

The g' and f' are given by the series expansion [3]

$$g' = \sum_m a_m x_o^m, \quad f' = \sum_m b_m x_o^m \quad (11a)$$

$$a_m = [- (\gamma - \gamma') a_{m-1} - (s_k + m + k) b_{m-1}] / [m(m + 2s_k)], \quad (12a)$$

$$b_m = [(s_k + m - k) a_{m-1} - (\gamma + \gamma') b_{m-1}] / [m(m + 2s_k)],$$

$$b_o = (\gamma + \gamma') / (k + s_k), \quad a_o = 1$$

In Eq. (12a) the superscripts R and I and the subscripts k have been omitted for the sake of clarity.

The normalization coefficients N are obtained by comparing the G and F of Eq. (10a) with those given in terms of the hypergeometric functions [5],

$$N_k^{R,I} = - (k/|k|) 2^{s_k} \pi \gamma / 2 \left[\frac{k(k + s_k) + \gamma'(\gamma' - \gamma)}{2(k^2 + \gamma')} \right]^{\frac{1}{2}} \cdot$$

$$|\Gamma(s_k + 1 + i\gamma)| / [\Gamma(2s_k + 1)]. \quad (13a)$$

The ratio $(N^R/N^I)_k$ is most convenient in the form

$$(N^R/N^I)_k = \frac{|\Gamma(\rho_k + i\gamma)|^2}{|\Gamma(2\rho_k)|^2} \frac{(\rho_k^2 + \gamma^2)^{\frac{1}{2}}}{2\rho_k} \cdot \frac{X[\cos h^2(\pi\gamma) - \cos^2 \pi\rho_k]^{\frac{1}{2}}}{\sin 2\pi\rho_k} \quad (14a)$$

$$X 2^{2\rho_k} \left\{ [k(k + \rho_k) + \gamma'(\gamma' - \gamma)] / [k(k - \rho_k) + \gamma'(\gamma' - \gamma)] \right\}^{\frac{1}{2}}$$

$$\rho_k = |s_k|.$$

Finally, the scatterin amplitudes [5] $f(\theta)$ and $g(\theta)$, from which the cross section $\sigma(\theta)$ is obtained, are given in terms of the Legendre polynomials $P_k(\cos\theta)$ as

$$f(\theta) = (2i\kappa)^{-1} \sum_k c_k P_k$$

$$g(\theta) = (2i\kappa \sin\theta)^{-1} \sum_k d_k P_k \quad (15a)$$

$$c_k = (2k + 1)(e^{i\eta_{k+1}} - 1) + k\alpha_k$$

$$d_k = [(k+1)(k+2)\alpha_{k+1}/(2k+3)] - k(k-1)\alpha_{k-1}/(2k-1) \quad (16a)$$

$$\alpha_k = e^{2i\eta} - |k| - e^{2i\eta}_{k+1}$$

$$\sigma(\theta) = |f(\theta)|^2 + |g(\theta)|^2$$

18000
28000
38000
48000
58000
68000
78000
88000
98000
108000
118000
128000
138000
148000
158000
168000
178000
18000
19000
20000
21000
22000
23000
24000
25000
26000
27000
28000
29000
30000

THIS PROGRAM IS USED TO CALCULATE SCATTERING CROSS SECTIONS FOR ELECTRONS INCIDENT ON NUCLEI. THE METHODS USED ARE BASICALLY THOSE OF RAWITSCHER AND CAN BE FOUND IN VOLUME 112 NUMBER 4, PHYSICAL REVIEW, PAGE 1274. WHILE THERE IS MUCH DESCRIPTIVE COMMENT CONTAINED IN THIS PROGRAM, AN EVEN MORE DETAILED EXPLANATION OF THE METHODS USED CAN BE OBTAINED FROM PROFESSOR F. BUSKIRK, PHYSICS DEPARTMENT, NPS.

MOST OF THE COMMENTS CONTAINED HEREIN WILL PERTAIN TO ACTUAL USAGE OF THE PROGRAM, ESPECIALLY IN REGARD TO ITS MECHANICAL LIMITATIONS AND CAPABILITIES. A DETAILED SET OF COMMENTS IS PRESENT IN THE YALERF SUBPROGRAM DUE TO THE COMPLEXITY OF THE PROGRAM.

ALL THE COMMENTS CONTAINED IN THE PROGRAM PERTAIN TO THE STEP OR SET OF STEPS IMMEDIATELY PRECEDING THEM.

THIS IS THE MAIN CONTROL PROGRAM FOR YALERF. IT CONTROLS THE INPUT AND OUTPUT. THE PROGRAM HAS 11 INPUT PARAMETERS WHICH ARE CONTAINED ON 2 CARDS. THESE PARAMETERS, WITH FORMAT AND UNITS ARE AS FOLLOWS:

SYMBOL	DESCRIPTION	FORMAT	UNITS
CARD 1			
Z	NUCLEAR CHARGE	F10.5	DIMENSIONLESS
A	ATOMIC WEIGHT	F10.5	DIMENSIONLESS
P1	1ST PARAMETER	F10.5	SEE BELOW
P2	2ND PARAMETER	F10.5	SEE BELOW
P3	3RD PARAMETER	F10.5	SEE BELOW
MODEL	CHARGE DISTRIBUTION	I10	DIMENSIONLESS
CARD 2			
EO	INCIDENT ELECTRON ENERGY	F10.5	MEV
T1	INITIAL ANGLE	F10.5	DEG
T2	FINAL ANGLE	F10.5	DEG
TH	ANGLE STEP	F10.5	DEG
RO	FITTING ON RADIUS	F10.5	FM

EXPLANATION OF PARAMETERS:
VARIABLE CHARGE DISTRIBUTION TYPE
FERMI 1 GAUSSIAN(P-SHELL)
MODEL 2
P1 C(FM) A(FM)
P2 T(FM) ALPHA
P3 -

THE PROGRAM CAN CONTAIN HAS MANY DIFFERENT CHARGE DISTRIBUTIONS





DIMENSION	SIGMTC(100),RATIO(100),SIGCM(100),THCM(100)	000
COMMON S(950),S1(950),SLOC(950)		001
COMMON SLOC1(950)		002
COMMON EPHI(950),EPP(950),EPPP(950)		003
C		
1	READ(5,9000)Z,A,P1,P2,P3,MODEL	007
9000	FORMAT(5F10.5,I10)	008
	IF(Z)2,999,2	009
2	CONTINUE	010
	DO10J=1,100	011
9010	READ(5,9010)EO,T1,T2,TH,RO	012
	FORMAT(5F10.5)	013
	IF(EO)3,1,3	014
3	CONTINUE	015
	WRITE(6,9020) Z,A,MODEL,P1,P2,P3,EO,RO	016
9020	FORMAT(28H1ELASTIC ELECTRON SCATTERING /14H CROSS SECTION//	017
	14H Z =,F10.5/4H A =,F10.5/4H M =,I10/4H P1=,F10.5/4H P2=,F10.5/	018
	24H P3=,F10.5/4H EO=,F10.5//4H RO=,F10.5//)	019
	WRITE(6,9030)	020
9030	FORMAT(16,'THETA',T19,'SIGMA',T32,'SIGMA(MOTT)',T49,'FORMFACTOR')	021
	T=T1	022
	DO40L=1,100	023
C		1A023
C	THIS INDICATES THAT UP TO 100 ANGLE STEPS MAY BE USED IF DESIRED.	2A023
C		3A023
	THEXX(L)=T	024
	IF(T-T2)50,30,30	025
50	T=T+TH	026
40	CONTINUE	027
30	JMAX=L	028
C		1A028
C	JMAX IS EQUAL TO THE NUMBER OF SCATTERING ANGLES THAT CALCULATIONS	2A028
C	WILL BE DONE FOR.	3A028
C	CALL SIGTRU(EO,ECM,THEXX,THCM,JMAX,A,Z,MODEL,P1,P2,P3,RO,SIGTX,	4A028
	1SIGCM,SIGMTX,SIGMTC,FELSXX,RATIO)	029
C		030
C	THE SUBPROGRAM SIGTRU IS CALLED AND ALL PARAMETERS TRANSFERRED	1A030
C	TO IT ARE INDICATED. THE VARIABLE AND ARRAY NAMES USED IN SIGTRU	2A030
C	FOR THESE PARAMETERS ARE NOT NECESSARILY THE SAME. THIS WAS DONE	3A030
C	TO PROVIDE CLARITY WHILE FORMING COMPLETE PROGRAM. WHEREVER	4A030
C	POSSIBLE,VARIABLE AND ARRAY NAMES ARE USED WHICH ABBREVIATE	5A030
C	ACTUAL QUANTITY IN THEORETICAL WORK.	6A030
C		7A030
C		8A030
	DO20L=1,JMAX	031
20	WRITE(6,9040)THEXX(L),SIGMTX(L),FELSXX(L)	032
9040	FORMAT(F10.5,3E16.5)	033
10	CONTINUE	034



999 STOP
END

035
036

SUBROUTINE SIGTRU(E1,E1CM,TL,TCM,JM,AM,Z,MOD,C,T,W,FITRAD,SIGLAB,
1SIGCM,SIGMTL,SIGMTC,FELS,RATIO)
DIMENSION TL(100),TCM(100),RATIO(100),SM(100),FELS(100),
1SIGLAB(100),SIGCM(100),SIGMTL(100),SIGMTC(100)

SIG000010
SIG000020
SIG000030
SIG000040
1AS40
2AS40
3AS40
4AS40
5AS40
6AS40
7AS40

THIS IS THE SUBPROGRAM USED FOR THE TRANSFORMATION FROM CENTER
OF MASS COORDINATE SYSTEM, IN WHICH CALCULATIONS ARE DONE, TO
LAB. SYSTEM OF COORDINATES. THIS TRANSFORMATION IS DONE ACCORDING
TO THE RELATIONS IN THE ARTICLE BY DEDRICK, REVIEWS OF MODERN
PHYSICS, VOLUME 34, NUMBER 3, PAGE 429.

EM2=AM*931.478
EM1=.51106
ETCM=SQRT((EM1**2+EM2**2+2.*E1*EM2)
E1CM=(ETCM**2+EM1**2-EM2**2)/(2.0*ETCM)

SIG000080
SIG000090
SIG000100
SIG000110
1AS110
2AS110
3AS110

E1CM IS THE INCIDENT ENERGY OF ELECTRON IN CM FRAME.

A=(E1+EM1**2/EM2)/(E1+EM2)
G=(E1+EM2)/ETCM
CK=1.0-A*A
DO 40 I=1,JM

SIG000120
SIG000130
SIG000140
SIG000150
0AS150
1AS150
2AS150
3AS150

SINCE JM=JMAX IN PHASE, WE CALCULATE ANGLE IN CM FRAME FOR EACH
ANGLE IN LAB FRAME FOR WHICH RESULTS ARE DESIRED.

PHI=TL(I)*3.1415926/180.
CS=COS(PHI)
SN=SIN(PHI)
AN=CS*SQRT(G*G*CK*SN**2+CS**2)-1.0*A*G*G*SN**2
AD=G*G*SN**2+CS**2
COSPH=AN/AD
THCM=ARCCOS(COSPH)
TCM(I)=THCM*180./3.1415926

SIG000160
SIG000170
SIG000180
SIG000190
SIG000200
SIG000210
SIG000220
SIG000230

THIS IS ARRAY OF ANGLES IN CM FRAME CORRESPONDING TO GIVEN LAB
FRAME ANGLES.

A1=G*G*CK*SN**2+CS**2
A2=1.0-2.0*CS**2
TOP=AD*(G*G*CK*A2+2.0*CS**2)
TOP=TOP+2.0*(G*G*A*SQRT(A1)-(1.0-G*G)*A1)*CS
BOT=AD**2*SQRT(A1)
40 RATIO(I)=TOP/BOT

1AS230
2AS230
3AS230
4AS230
SIG000240
SIG000250
SIG000260
SIG000270
SIG000280
SIG000290

CCCC CCCCC

THIS IS THE FACTOR WHICH MULTIPLIES CROSS SECTIONS CALCULATED IN
CM FRAME TO GIVE CROSS SECTIONS IN LAB FRAME.

CALL YALERF(EICM,TCM,JM,AM,Z,MOD,C,T,W,FITRAD,SIGCM,SIGMTC,FELS)

THE SURPROGRAM YALERF IS CALLED AND ALL PARAMETERS TRANSFERRED
TO IT ARE INDICATED. THE YALERF SUBPROGRAM IS WHERE ALL CROSS
SECTION CALCULATIONS ARE DONE.

DO 50 I=1,JM
SIGMTL(I)=SIGMTC(I)*RATIO(I)
SIGLAB(I)=SIGCM(I)*RATIO(I)
FELS(I)=SIGLAB(I)/SIGMTL(I)
CONTINUE
RETURN
END

50

SUBROUTINE YALERF(EINCX,THEXX,LXXXXX,AXXX,ZXXXX,MODEL,C,TXXXX,WXX
1XX,FITRAD,SIGTX,SIGMTX,FELSSX)
COMMON S(1100),SI(1100),SLOC(1100)
COMMON EPHI(1100), EPP(1100), EPPP(1100)
COMMON PRECISION A,FR,GR,FI,GI,SVOFK,ALPHA,ALPHA2,EALP,PUC2
DOUBLE PRECISION PUC,TEMP,BETA,GM,SQB,GP,CK,GGP,PHIK,S
DOUBLE PRECISION XO,X1,ZKR,ZKI,ANR1,ANR1,BNR1,DOMR,DOMI
DOUBLE PRECISION FRNEG,GINEG,XFI,XGR,XGI,T
DOUBLE PRECISION ANR,BNR,ANI,BNI, GRP,FRP,FIP,GIP,GRNEG
SQS(X,Y)=X**2+Y**2
CSHY(X)=(EXP(X)+EXP(-X))/2.
SSHY(X)=(EXP(X)-EXP(-X))/2.
GAM1(X,Y)=(X-5)*.5*ALOG(SQS(X,Y))-Y*ATAN(Y/X)-X+.5*ALOG(6.2831
185)+X/(12.*SQS(X,Y))-(X**3-3.*Y**2**X)/(1260.*SQS(X,Y)**3)
2+(X**5-10.*X**3*Y**2+5.*X*Y**4-7.*X**Y**6)/(1680.*SQS(X,Y)**7)
3*5*Y**2+35.*X**3*Y**4-7.*X*Y**6)/(1680.*SQS(X,Y))-2.*Y-Y/(6.*S
1QS(X,Y))=5*(X-5)*.5*ATAN(Y/X)+Y*ALOG(SQS(X,Y))
2-((5.*Y*X**4-10.*Y**3*X**2+Y**5)/(1260.*SQS(X,Y)**5))
3+((Y*(7.*X**6-35.*X**4*Y**2+21.*X**2*Y**4-Y**6))/(1680.*SQS(X,Y)*
4*7))
GAM4(X,Y)=-ATAN(Y/X)-ATAN(Y/(X+1))-ATAN(Y/(X+2))*GAM3((X+3.
1),Y)
1DIMENSION Y(3),Y1(3),Y2(3),
AX(4),AA(4),B(4),BA(4),
12AM(4),ANM(4),PM(4),ETAKP(140),ETAKN(140),ETKP(140),ETKN(140),COR(1
340,5),COI(140,5),ALR(140),ALI(140),DOR(140,5),
4ZP(140),F(600),G(600),DOI(140,5),ATA(140),ETI(140)


```

C      DIMENSION A(25),FR(600),GR(600),FI(600),GI(600)
C      DIMENSION THEXX(100),SIGTXX(100),SIGMTX(100),FELSXX(100)
C      IN THIS SUBPROGRAM,BEFORE CALCULATIONS CAN BE MADE IT IS NECESSARY
C      TO PUT ALL QUANTITIES IN DIMENSIONLESS FORM APPROPRIATE TO COM-
C      PUTER CALCULATIONS. ALSO,SEVERAL VALUES OF CONSTANTS NEEDED ARE
C      CALCULATED FIRST.
C      EINCX=EINCX-0.5110
C      EINCX=KINETIC ENERGY OF ELECTRON IN CM FRAME.
C      6001
C      A(3) = EINCX
C      A(1) = AXXXX
C      A(2) = ZXXXXX
C      A(4) = 0.511
C      A(5) = C/(A(1)**.3333333)
C      A(6) = TXXXX
C      A(7) = 0.0
C      A(8) = 1.0
C      A(9) = 0.729729D-02
C      A(10) = 0.38615D+03
C      A(11) = 0.15625D-01
C      A(12) = 0.1953125D-02
C      A(13) = 0.1D-09
C      A(14) = 0.1D-09
C      A(15) = 0.0
C      A(16) = A(12)
C      A(17) = 0.1D-05
C      A(18) = 0.0
C      A(19) = 1.0D0
C      A(20) = 1.0
C      A(21) = 1.0
C      A(22) = 0.0
C      A(23) = 0.0
C      A(24) = 1.0
C      OF ABOVE VALUES,SOME WERE INITIALLY USED IN TEST RUNS AND IN
C      DEBUGGING PROCEDURES, AND ARE NOT USED IN FINAL PROGRAM.
C      LAG=34
C      LAG VALUE CONTROLS UPPER LIMIT ON SUMMATIONS OVER ANGULAR
C      MOMENTUM QUANTUM NUMBER K(SVOFK IN PROGRAM) CARRIED OUT IN
C      LATER CALCULATIONS.
C      125
C      CONTINUE
C      SVOFK=1.

```

```

YAL000300
YAL000310
1AY310
2AY310
3AY310
4AY310
5AY310
6AY310
YAL000320
1AY320
2AY320
3AY320
YAL000330
YAL000340
YAL000350
YAL000360
YAL000370
YAL000380
YAL000390
YAL000400
YAL000410
YAL000420
YAL000430
YAL000440
YAL000450
YAL000460
YAL000470
YAL000480
YAL000490
YAL000500
YAL000510
YAL000520
YAL000530
YAL000540
YAL000550
YAL000560
1AY560
2AY560
3AY560
4AY560
YAL000570
1AY570
2AY570
3AY570
4AY570
5AY570
YAL000580
YAL000590

```


CCCC CCCC CCCC CCCC CCCC CCCC CCCC C

THE INITIAL VALUE OF ANGULAR MOMENTUM QUANTUM NUMBER K IS SET
EQUAL TO +1.

ALPHA=A(2)*A(9)

THIS IS ALPHA DEFINED IN APPENDIX OF RAWITSCHER'S ARTICLE.

ALPHA2=ALPHA**2
EALP=A(8)*ALPHA
PUC2=((2.+A(3))/A(4))*A(3))/A(4)
PUC = DSQRT(PUC2)

THIS IS MOMENTUM OF INCIDENT ELECTRON IN DIMENSIONLESS UNITS.

TEMP=1.+A(3)/A(4)
BETA=PUC/TEMP

THIS IS BETA DEFINED IN APPENDIX OF RAWITSCHER'S ARTICLE.

GM=EALP/BETA

THIS IS GAMMA DEFINED IN APPENDIX OF RAWITSCHER'S ARTICLE.

SOB=1./TEMP
GP=GM*SQB

THIS IS PRIMED GAMMA IN APPENDIX OF RAWITSCHER'S ARTICLE.

CK=PUC/A(10)

THIS IS KAPPA IN APPENDIX OF RAWITSCHER'S ARTICLE.

XO=FITRAD*CK

THIS IS MATCHING RADIUS IN DIMENSIONLESS UNITS. NOTE THAT IF
NEW STEPS ARE PLACED ANYWHERE IN PROGRAM, ALL QUANTITIES WHICH
ARE LINEAR DISTANCES (IN FERMI'S) MUST BE MULTIPLIED BY CK
TO GIVE CORRECT RESULTS.

LOP=1

THIS IS A RUNNING INDEX WHICH IS USED LATER IN CONJUNCTION WITH
SUMMING OVER ANGULAR MOMENTUM QUANTUM NUMBERS.

CP=C*CK

Z1P=(A(6)/4.3944)*CK

1AY590
2AY590
3AY590
4AY590
YAL00600
1AY600
2AY600
3AY600
YAL00610
YAL00620
YAL00630
YAL00640
1AY640
2AY640
3AY640
YAL00650
YAL00660
1AY660
2AY660
3AY660
YAL00670
1AY670
2AY670
3AY670
YAL00680
YAL00690
1AY690
2AY690
3AY690
YAL00700
1AY700
2AY700
3AY700
YAL00740
1AY740
2AY740
3AY740
4AY740
5AY740
6AY740
YAL00750
1AY750
2AY750
3AY750
4AY750
YAL00760
YAL00770
1AY770


```

CC      THESE ARE 2 CHARGE DISTRIBUTION PARAMETERS IN DIMENSIONLESS UNITS.      2AY770
CC      E1P=(2.+A(3)/A(4))/PUC      3AY770
CC      EMIP=(A(3)/A(4))/PUC      YAL00780
CC      GGP=ALPHA2/(GM+GP)      YAL00790
CC      REFER TO NOTES HELD BY PROF. BUSKIRK FOR ABOVE 3 STEPS.      YAL00800
CC      WE NOW CALCULATE THE CHARGE DENSITY AND RESULTING POTENTIAL AT      1AY800
CC      INCREMENTAL STEPS OUT TO MATCHING RADIUS. THE INTEGRATION IS DONE      2AY800
CC      USING SIMPSONS RULE. THE INCREMENTAL STEP VALUES USED ARE THE      3AY800
CC      SAME AS THOSE THAT WILL BE USED IN LATER NUMERICAL INTEGRATION      4AY800
CC      OF RADIAL WAVE EQUATIONS.      5AY800
CC      6AY800
CC      7AY800
CC      8AY800
CC      9AY800
CC      10AY800
CC      11AY800
CC      YAL00840
CC      YAL00850
CC      1AY850
CC      2AY850
CC      3AY850
CC      4AY850
CC      YAL00860
CC      YAL00870
CC      YAL00880
CC      1AY880
CC      2AY880
CC      3AY880
CC      4AY880
CC      5AY880
CC      YAL00890
CC      YAL00900
CC      1AY900
CC      2AY900
CC      3AY900
CC      4AY900
CC      YAL00910
CC      YAL00920
CC      YAL00930
CC      YAL00940
CC      YAL00950
CC      YAL00960
CC      YAL00970
CC      1AY970
CC      2AY970
CC      3AY970
CC      4AY970
CC      5AY970

```

REFER TO NOTES HELD BY PROF. BUSKIRK FOR ABOVE 3 STEPS.

WE NOW CALCULATE THE CHARGE DENSITY AND RESULTING POTENTIAL AT INCREMENTAL STEPS OUT TO MATCHING RADIUS. THE INTEGRATION IS DONE USING SIMPSONS RULE. THE INCREMENTAL STEP VALUES USED ARE THE SAME AS THOSE THAT WILL BE USED IN LATER NUMERICAL INTEGRATION OF RADIAL WAVE EQUATIONS.

```

20  RX=0
    M=0
    RX IS THE RADIAL DISTANCE FROM CENTER OF NUCLEUS AND M IS A
    RUNNING INDEX.
    GRID=A(12)/2.
    XFR=A(12)
    XN=A(12)
    GRID IS A SPACING DISTANCE BETWEEN POINTS WHERE CHARGE DENSITY
    AND DERIVATIVES ARE CALCULATED. XFR AND XN KEEP TRACK OF POINTS
    BETWEEN WHICH SIMPSONS RULE INTEGRATION WAS DONE.
    SUM2=0
    SUM3=0
    SUM2 AND SUM3 WILL BE USED TO STORE RESULTS FROM THE 2 INTEGRALS
    NECESSARY TO GET THE POTENTIAL V(RX).
    DO 25 J=1,1100
    DO23L=1,3
    Y(L)=FMOD(MODEL,RX,CK,C,TXXXX,WXXXX)
    Y1(L)=Y(L)*RX
    Y2(L)=Y1(L)*RX
    RX=RX+GRID
    21 CONTINUE
    23
    THESE STEPS CALCULATE THE VALUE OF THE CHARGE DENSITY AT RX AND
    ALSO RX*(CHARGE DENSITY) AND RX**2*(CHARGE DENSITY). THESE LAST
    2 QUANTITIES ARE THOSE WHICH MUST BE INTEGRATED TO GIVE V(RX).
    THE FUNCTION FMOD IS WHERE THE CHARGE DENSITY CALCULATIONS ARE

```



```

CC      DONE. THE J=1,3 PROVIDES FOR VALUES AT 3 SUCCEEDING POINTS.
C      RX=RX-GRID
C      S(J)=(Y1(1)+4.*Y1(2)+Y1(3))*GRID/3.
C      S1(J)=(Y2(1)+4.*Y2(2)+Y2(3))*GRID/3.
C      SLOC(J)=Y(3)
C      SLOC1(J)=Y2(3)
C      M=M+1
C      THE RESULTS FROM INNER DO LOOP ABOVE ARE USED TO INTEGRATE BY
C      SIMPSON'S RULE. SLOC(J) AND SLOC1(J) ARE USED TO STORE END POINT
C      OF INTEGRATION VALUES FOR FUTURE USE.
C      IF(J-1098)71,71,22
C      IF(RX-(X0+A(11)/2.))26,70,70
C      71
C      THE 1ST IF STATEMENT IS USED TO ENSURE THAT THE FITTING RADIUS
C      IS REACHED BEFORE INTEGRATION STOPS DUE TO END VALUE OF DO LOOP.
C      IT WORKS IN CONJUNCTION WITH 2ND IF STATEMENT WHICH ACTUALLY
C      CHECKS TO SEE IF X0 HAS BEEN REACHED WITHIN A GIVEN INTERVAL.
C      IF THE FITTING RADIUS HASN'T BEEN REACHED BY J=1098, THEN THE
C      NEXT RUN THROUGH DO LOOP WILL CAUSE 1ST IF TO TRANSFER TO 22
C      WHERE THE GRID SPACING IS DOUBLED AND THIS FACT IS PRINTED OUT.
C      THE ENTIRE SET OF CALCULATIONS IS THEN REPEATED FROM 125 ON.
C      NOTE THAT X0 IS FUNCTION OF MOMENTUM(DUE TO CK) AND HENCE AS
C      HIGHER INCIDENT ENERGIES ARE USED, FOR A GIVEN VALUE OF FITRAD,
C      X0 WILL INCREASE, ULTIMATELY CAUSING ABOVE DOUBLING OF SPACING
C      BETWEEN INTEGRATION STEPS. IF INCIDENT ENERGIES GREATER THAN
C      APPROXIMATELY 150 MEV ARE USED, THIS WILL OCCUR. TO PREVENT IT,
C      INCREASE J AND HENCE STORAGE REQUIREMENTS, AND/OR DECREASE FITRAD.
C      FOR INFORMATION PURPOSES, AN INCREASE IN J TO 1500 ALONG WITH A
C      FITRAD=8 FERMI'S WILL ALLOW FOR INTEGRATIONS WITH SAME SPACING
C      UP TO AN INCIDENT ENERGY OF APPROXIMATELY 250 MEV. THE RESULTS
C      OBTAINED IF SPACING IS DOUBLED ARE NOT INVALID BUT CAN'T BE
C      CORRELATED VERY WELL TO LOWER ENERGY RESULTS USING A DIFFERENT
C      SPACING.
C      26 IF(J-1)28,28,300
C      28 GRID=A(11)/4.
C      XFR=XFR+A(11)/2.
C      27 GOTO25
C      300 XFR=XFR+A(11)/2.
C      25 CONTINUE
C      A SMALLER SPACING IS USED FOR FIRST INTEGRATION IN ATTEMPT TO
C      GET ACCURATE STARTING POINT. IF(J-1) CAUSES THIS TO BE INCREASED

```

```

6AY970
7AY970
YAL00980
YAL00990
YAL01000
YAL01010
YAL01020
YAL01030
1AY1030
2AY1030
3AY1030
4AY1030
5AY1030
YAL01040
YAL01050
1AY1050
2AY1050
3AY1050
4AY1050
5AY1050
6AY1050
7AY1050
8AY1050
9AY1050
10AY1050
11AY1050
12AY1050
13AY1050
14AY1050
15AY1050
16AY1050
17AY1050
18AY1050
19AY1050
20AY1050
21AY105
22AY1050
23AY1050
24AY1050
YAL01060
YAL01070
YAL01080
YAL01090
YAL01100
YAL01110
1AY1110
2AY1110
3AY1110

```



```

C      AND SAME VALUE USED FOR ALL OTHER CALCULATIONS.
C      22  A(11)=A(11)*2.
          WRITE(6,7011)
7011  FORMAT(85H0 STORAGE CAPACITY HAS BEEN EXCEEDED.GRID IS MULTIPLIED BY
1Y 2 AND CALCULATION REPEATED.)
C      70  GO TO 125
          J=0
          DO 29 J=1,M
            SUM2=SUM2+S(J)
            XC=RX
            29  SUM3=SUM3+S1(J)
C      SUM2 AND SUM3 GIVE TOTAL AREAS UNDER CURVES AFTER COMPLETION OF
C      DO 29 J=1,M.
          DO 50 J=2,M
            S1(J)=S1(J)+S1(J-1)
            50  S(J)=S(J)+S(J-1)
C      AFTER COMPLETION OF THIS DO LOOP,EACH S(J) AND S1(J) CONTAINS
C      AREA UNDER CURVE FROM RX=0 TO ITS RELATED RX VALUE.
          DO 30 J=1,M
            EPHI(J)=(-EALP/SUM3)*(S1(J)/XN-S(J)+SUM2)
            EPP(J)=(EALP/XN*2)*(S1(J)/SUM3)
            SLOC(J)=SLOC(J)/SUM3
            SLOC1(J)=SLOC1(J)/SUM3
            30  XN=XN+A(11)/2.
C      EPHI(J) IS THE POTENTIAL V(RX) AND EPP(J) IS THE FIRST DERIVATIVE
C      OF THIS POTENTIAL. CERTAIN MANIPULATIONS OF V(RX) FORMULA ARE
C      NECESSARY BEFORE IT HAS ABOVE FORM. REFER TO NOTES HELD BY
C      PROF. BUSKIRK FOR THESE DETAILS.
C      NOTE THAT NORMALIZATION CONSTANTS FOR CHARGE DISTRIBUTIONS ARE
C      NOT NEEDED IN USE OF PROGRAM DUE TO DIVISION BY SUM3.
C      THE CHARGE DENSITIES HAVE BEEN USED TO CALCULATE THE POTENTIAL
C      AND ITS FIRST DERIVATIVE AT LOCATIONS FROM CENTER OF NUCLEUS
C      OUT TO FITTING-ON RADIUS. WITH THIS DATA WE CAN NOW PROCEED TO
C      CALCULATE THE VALUES OF THE REGULAR AND IRREGULAR COULOMB FUNC-
C      TIONS AT THE FITTING-ON OR MATCHING RADIUS.
          10  PHIK=DSQRT(SV0FK**2-ALPHA2)
              ASSIGN 80 TO JACK
          80  YAL01110
              5AY1110
              YAL011120
              YAL011130
              BYAL011140
              YAL011150
              YAL011160
              YAL011170
              YAL011180
              YAL011190
              YAL011200
              YAL011210
              1AY11210
              2AY11210
              3AY11210
              4AY11210
              YAL011220
              YAL011230
              YAL011240
              1AY11240
              2AY11240
              3AY11240
              4AY11240
              YAL011250
              YAL011260
              YAL011270
              YAL011280
              YAL011290
              YAL011300
              1AY11300
              2AY11300
              3AY11300
              4AY11300
              5AY11300
              6AY11300
              7AY11300
              8AY11300
              9AY11300
              10AY11300
              11AY11300
              12AY11300
              13AY11300
              14AY11300
              15AY11300
              16AY11300
              17AY11300
              YAL011340
              YAL011350

```


C
C
C

PHIK IS S-SUB-K IN APPENDIX OF RAWITSCHER'S ARTICLE.

32

T=1.0
IF(A(16)-A(18))325,325,640
IF(A(16)-XO)642,645,645
640 A(16)=A(16)+A(11)
642 GOTO 640
645 A(16)=A(16)-A(11)
325 X1=A(16)

C
C
C
C
C
C
C
C

THE FIRST IF STATEMENT ABOVE IS USED AS A WAY OF LEAVING A(16) AT ITS INITIAL VALUE. THE SECOND IF STATEMENT COMPARES A(16) WITH XO. IF A(16) IS LESS THAN XO, AS IT NORMALLY WOULD BE, THEN THE NEXT SERIES OF STEPS INCREMENT UP UNTIL IT IS A(11) LESS THAN XO. NOTE THAT AT YAL01200 XO WAS SET=RX, WHERE RX WAS THEN THE CLOSEST POINT OF INTEGRATION RESULTS TO ORIGINAL XO. X1 IS SET=THIS FINAL VALUE OF A(16).

11

N=1
IF(SVOFK)11,12,12
ZKR=ALPHA2/(SVOFK-PHIK)
ZKI=SVOFK-PHIK

16

ANR1=1.
ANR1=(GM+GP)/ZKR
BNR1=(GM+GP)/ZKI
XFR=ANR1
XFI=ANR1
XGR=BNR1
XGI=BNR1

15

DOMR=T*(T-2.*SVOFK+2.*ZKR)
ANR=(-GGP*ANR1-T*(T-2.*SVOFK+2.*ZKR))
BNR=((ZKR+T-2.*SVOFK)*ANR1-(GM+GP)*BNR1)*X1/DOMR
BNI=(-GGP*ANR1-T*(T-2.*SVOFK+2.*ZKR))
ANI=((ZKI+T-2.*SVOFK)*ANR1-(GM+GP)*BNR1)*X1/DOMR
IF(N-1)13,13,14

13

XFR=XFR+ANR
XFI=XFI+ANI
XGR=XGR+BNR
XGI=XGI+BNI
N=N+1
T=T+1.
ANR1=ANR
ANI1=ANI
BNR1=BNR
BNI1=BNI

1AY1350
2AY1350
3AY1350
YAL01350
YAL01370
YAL01380
YAL01390
YAL01400
YAL01410
YAL01420
1AY1420
2AY1420
3AY1420
4AY1420
5AY1420
6DY1420
7AY1420
8AY1420
9AY1420
YAL01430
YAL01440
YAL01450
YAL01460
YAL01470
YAL01480
YAL01490
YAL01500
YAL01510
YAL01520
YAL01530
YAL01540
YAL01550
YAL01560
YAL01570
YAL01580
YAL01590
YAL01600
YAL01610
YAL01620
YAL01630
YAL01640
YAL01650
YAL01660
YAL01670
YAL01680
YAL01690
YAL01700
YAL01710

H2=A(11)/2.
H210=A(11)**2/12.

K=1
L=2
X=A(12)-EM1P*EALP*SUM2/SUM3
AO=-1.+E1P*EALP*SUM2/SUM3
BO=1.+E1P*EALP*SUM2/SUM3
IF(SVOFK)60,61,61
61 B1L=BO/(2.*DABS(SVOFK)+1.)
F(1)=X*B1L
G(1)=1.
GOTO 62
60 A1L=AO/(2.*DABS(SVOFK)+1.)
F(1)=1.
G(1)=X*A1L

THE ABOVE STEPS CALCULATE THE INITIAL VALUES OF THE RADIAL WAVE
FUNCTIONS AT X=A(12), WHERE A(12) WAS EARLIER STARTING POINT FOR
V(R) CALCULATIONS. THE SERIES EXPANSION USED FOR THE INITIAL
VALUES OF F(1) AND G(1) IS FROM THE ARTICLE BY WOLFGANG BUHRING,
Z. PHYSIK, VOLUME 187, P. 183. THE INTERNAL REGION IN THE SERIES
IS USED, KEEPING ONLY THE FIRST NON-ZERO TERM IN THE SIGN OF
VALUE OF THIS TERM FOR F(1) OR G(1) DEPENDS ON THE SIGN OF SVOFK.

62 EPO=EPI(1)
EPI=EPP(1)
35 DO34J=1,4
AA(J)=AX(J)
VP=0
VPI=0

34 BA(J)=B(J)
V1=(EPO-VP)*EM1P
V2=(EPO-VP)*E1P
V1P=(EPI-VP1)*EM1P
V2P=(EPI-VP1)*E1P
AX(1)=-SVOFK/X
AX(2)=1.-V2
AX(3)=-1.+V1
AX(4)=SVOFK/X
B(1)=SVOFK*(SVOFK+1.)/X**2-(1.-V2)*(1.-V1)
B(2)=-V2P
B(3)=V1P
B(4)=SVOFK*(SVOFK-1.)/X**2-(1.-V1)*(1.-V2)
X=X+A(11)
DO33J=1,4
AX(J)=AX(J)*H2
B(J)=B(J)*H210
33 B(1)=1.+B(1)

CCCCCCCC

YAL01970
YAL01980
YAL01990
YAL02000
YAL02010
YAL02020
YAL02030
YAL02040
YAL02050
YAL02060
YAL02070
YAL02080
YAL02090
YAL02100
YAL02110
1AY2110
2AY2110
3AY2110
4AY2110
6AY2110
6AY2110
7AY2110
8AY2110
9AY2110
YAL02120
YAL02130
YAL02140
YAL02150
YAL02160
YAL02170
YAL02180
YAL02190
YAL02200
YAL02210
YAL02220
YAL02230
YAL02240
YAL02250
YAL02260
YAL02270
YAL02280
YAL02290
YAL02300
YAL02310
YAL02320
YAL02330
YAL02340
YAL02350

YAL02360
YAL02370
YAL02380
YAL02390
YAL02400
YAL02410
YAL02420
YAL02430
YAL02440
YAL02450
YAL02460
YAL02470
YAL02480
YAL02490
YAL02500
YAL02510
YAL02520
YAL02530
YAL02540
YAL02550
YAL02560
YAL02570
YAL02580
YAL02590
YAL02600
YAL02610
YAL02620
YAL02630
YAL02640
YAL02680
1AY2680
2AY2680
3AY2680
5AY2680
5AY2680
6AY2680
7AY2680
8AY2680
9AY2680
10AY2680
YAL02690
YAL02700
YAL02710
YAL02720
YAL02730
YAL02740
1AY2740
2AY2740

```

37 B(4)=1.+B(4)
   K=K+2
   EPO=EPP(K)
   EPI=EPP(K)
   GOTO N, (37,36)
38 ASSIGN 36 TO N
   GOTO 35
36 D(38J)=1,4
   AM(J)=AA(J)+RA(J)
   ANM(J)=B(J)-AX(J)
   DEN=ANM(1)*ANM(4)-ANM(2)*ANM(3)
   PM(1)=AM(1)*ANM(4)-AM(3)*ANM(2)
   PM(2)=AM(2)*ANM(4)-AM(4)*ANM(2)
   PM(3)=AM(3)*ANM(1)-AM(1)*ANM(3)
   PM(4)=AM(4)*ANM(1)-AM(2)*ANM(3)
   F(L)=(PM(1)*F(L-1)+PM(2)*G(L-1))/DEN
   G(L)=(PM(3)*F(L-1)+PM(4)*G(L-1))/DEN
   L=L+1
   IF(X-X0)35,40,40
40 LMAX=L-1
   IF(LAG-250)691,695,695
695 CONTINUE
691 GOTO JACK,(200,203)
200 GPP=G(LMAX)
   FPP=F(LMAX)
   SVOFK=-SVOFK
   ASSIGN 203 TO JACK
   GO TO 207
203 ASSIGN 204 TO JACK
205 ASSIGN 47 TO N

```

CCCCCCCCCCCC

THE ABOVE STEPS ARE FOR THE INTEGRATION OF THE RADIAL WAVE
FUNCTIONS OUT TO THE FITTING RADIUS. THE INTEGRATION PROCEDURE
IS THAT OF YENNIE, RAVENHALL, AND WILSON, AND IS OUTLINED IN THE
PHYSICAL REVIEW, VOLUME 95, NUMBER 2, P. 511. IN RELATION TO THIS,
ONLY DERIVATIVES UP TO 2ND WERE USED HERE. THE INTEGRATION IS
DONE FOR BOTH +AND- VALUES OF SVOFK. AFTER COMPLETION OF THIS
INTEGRATION PROCEDURE, GPP AND FPP WILL CONTAIN FINAL VALUES
FOR + SVOFK AND G(LMAX) AND F(LMAX) HAVE VALUES FOR - SVOFK.

```

K=1
H2=A(11)/2.
H210=A(11)*2/12.
X=A(16)
L=2
IF(X0-A(16)-3.*A(11))321,321,45

```

CC

AT THIS POINT, A CHECK IS MADE TO DETERMINE IF INTEGRATION OF


```

C      COULOMB FUNCTIONS FROM PREVIOUS X1 TO X0 IS NECESSARY. THIS IS
C      DETERMINED BY ABOVE IF STATEMENT. DUE TO SPACING USED IN NUMBER-
C      ICAL INTEGRATION OF RADIAL WAVE FUNCTIONS, VALUE OF X0, AND VALUE
C      OF X1, FURTHER INTEGRATION MAY BE NECESSARY OVER THIS SMALL RANGE.
321  LMAXIR=1
      GR(LMAXIR)=GRP
      FR(LMAXIR)=FRP
      GI(LMAXIR)=GIP
      FI(LMAXIR)=FIP
      GRN=GRNEG
      FRN=FRNEG
      GIN=GINEG
      FIN=FINEG
      GO TO 206

C      INDEPENDENT OF WHETHER FURTHER INTEGRATION IS DONE OR NOT, GR(1),
C      FR(1), GI(1), AND FI(1) CONTAIN VALUES OF REGULAR AND IRREGULAR
C      COULOMB WAVE FUNCTIONS FOR + SVOFK. GRN, FRN, GIN CONTAIN
C      CORRESPONDING VALUES FOR - SVOFK. IF INTEGRATION IS DONE, THE
C      RESULTS ARE PUT IN THESE VARIABLE NAMES BY LATER STEPS. THIS
C      IS NECESSARY SINCE INITIAL SVOFK SIGN IS - FOR FURTHER INTE-
C      GRATION ROUTINE.
45  EPC=-EALP/X
      EPI=EALP/X**2
      DD44J=1,4
      AA(J)=AX(J)
      BA(J)=B(J)
      V1=(EPO-VP)*EM1P
      V2=(EPO-VP)*E1P
      V1P=(EPI-VP1)*EM1P
      V2P=(EPI-VP1)*E1P
      AX(1)=-SVOFK/X
      AX(2)=1.-V2
      AX(3)=-1.+V1
      AX(4)=SVOFK/X
      B(1)=SVOFK*(SVOFK+1.)/X**2-(1.-V2)*(1.-V1)
      B(2)=-V2P
      B(3)=V1P
      B(4)=SVOFK*(SVOFK-1.)/X**2-(1.-V1)*(1.-V2)
      X=X+A(1)
      DD43J=1,4
      AX(J)=AX(J)*H2
      B(J)=B(J)*H210
      B(1)=1.+B(1)
      B(4)=1.+B(4)
      GOTO N,(47,46)
43
3AY2740
4AY2740
5AY2740
6AY2740
7AY2740
YAL02750
YAL02760
YAL02770
YAL02780
YAL02790
YAL02800
YAL02810
YAL02820
YAL02830
YAL02840
1AY2840
2AY2840
3AY2840
4AY2840
5AY2840
6AY2840
7AY2840
8AY2840
9AY2840
YAL02850
YAL02860
YAL02870
YAL02880
YAL02890
YAL02900
YAL02910
YAL02920
YAL02930
YAL02940
YAL02950
YAL02960
YAL02970
YAL02980
YAL02990
YAL03000
YAL03010
YAL03020
YAL03030
YAL03040
YAL03050
YAL03060
YAL03070
YAL03080

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47 ASSIGN 46 TO N
48 GO TO 45
49 DO 48 J=1,4
50 AM(J)=AA(J)+BA(J)
51 ANM(J)=B(J)-AX(J)
52 DEN=ANM(1)*ANM(4)-ANM(2)*ANM(3)
53 PM(1)=AM(1)*ANM(4)-AM(3)*ANM(2)
54 PM(2)=AM(2)*ANM(4)-AM(1)*ANM(3)
55 PM(3)=AM(3)*ANM(1)-AM(2)*ANM(4)
56 PM(4)=AM(4)*ANM(1)-AM(3)*ANM(2)
57 FR(L)=(PM(1)*FR(L-1)+PM(2)*GR(L-1))/DEN
58 CR(L)=(PM(3)*FR(L-1)+PM(4)*GR(L-1))/DEN
59 FI(L)=(PM(1)*FI(L-1)+PM(2)*GI(L-1))/DEN
60 GI(L)=(PM(3)*FI(L-1)+PM(4)*GI(L-1))/DEN
61 L=L+1
62 IF(X-X0)45,50,50
63 LMAXIR=L-1
64 GO TO JACK,(204,206)
65 GRN=GR(LMAXIR)
66 GIN=GI(LMAXIR)
67 FRN=FR(LMAXIR)
68 FIN=FI(LMAXIR)
69 GR(1)=GRP
70 GI(1)=GIP
71 FR(1)=FRP
72 FI(1)=FIP
73 SVOFK=DABS(SVOFK)
74 ASSIGN 206 TO JACK
75 GO TO 205
76 THE ABOVE STEPS ARE FOR THE INTEGRATION, IF NECESSARY, OF THE
77 COULOMB WAVE FUNCTIONS. THE INTEGRATION PROCEDURE IS THE SAME
78 AS WAS EARLIER USED FOR RADIAL WAVE FUNCTIONS. THE ONLY MAJOR
79 DIFFERENCE IS THAT THE POTENTIAL USED HERE IS THAT FOR A POINT
80 NUCLEUS.
81 206 STEAM=DEXP(GAM1(PHIK,GM)-GAM1(2.0*PHIK,0)+PHIK*DLOG(A(16)))
82 TYRE=STEAM**2
83 TEMP=TYRE*(
84 1 SQRT(SQS(PHIK,GM))/(2.0*PHIK))* (DSQRT((CSHY(3.141593*GM))**2-(DCO
85 2 S(3.141593*PHIK))**2)/DSIN(6.283185*PHIK)),
86 1 TEMP1=((GM+GP)*(DABS(SVOFK)+PHIK)/((DABS(SVOFK)*GM-GP*PHIK)*ALPHA2
87 1 ))*(DABS(SVOFK)*(DABS(SVOFK)+PHIK)-GP*ALPHA2/(GM+GP))
88 SVOFK=DABS(SVOFK)
89 RNINP=TEMP*SQRT(TEMP1)**2.0*(2.0*PHIK)
90 RNINN=((TEMP/SQRT(TEMP1))**2.0*(2.0*PHIK)
91 ASSIGN 800 TO JACK
92 DCKP=((GR(LMAXIR)-(GPP/FPP)*FR(LMAXIR))/((GPP/FPP)*FI(LMAXIR)-GI(

```

```

YAL03090
YAL03100
YAL03110
YAL03120
YAL03130
YAL03140
YAL03150
YAL03160
YAL03170
YAL03180
YAL03190
YAL03200
YAL03210
YAL03220
YAL03230
YAL03240
YAL03250
YAL03260
YAL03270
YAL03280
YAL03290
YAL03300
YAL03310
YAL03320
YAL03330
YAL03340
YAL03350
YAL03360
YAL03370
YAL03380
YAL03390
YAL03400
YAL03410
YAL03420
YAL03430
YAL03440
YAL03450
YAL03460
YAL03470
YAL03480
YAL03490
YAL03500
YAL03510
YAL03520

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CCCCCCCC


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1 LMAXIR)))#RNINP
DCKN=((GRN-(G(LMAX)/F(LMAX))*FRN)/((G(LMAX)/F(LMAX))*FIN-GIN))*
IRNINN
YAL03530
YAL03540
YAL03550
1AY3550
2AY3550
3AY3550
4AY3550
5AY3550
6AY3550
7AY3550
8AY3550
9AY3550
10AY3550
11AY3550
12AY3550
13AY3550
14AY3550
YAL03590
YAL03600
YAL03610
YAL03620
YAL03630
YAL03640
YAL03650
YAL03660
YAL03670
YAL03680
YAL03690
YAL03700
YAL03710
YAL03720
YAL03730
YAL03740
YAL03750
YAL03760
YAL03770
YAL03780
YAL03790
YAL03800
YAL03810
YAL03820
YAL03830
YAL03840
YAL03850
YAL03860
YAL03870
YAL03880
YAL03890

THE ABOVE STEPS CALCULATE THE RATIO(D/C), WHERE D AND C ARE THE
MATCHING COEFFICIENTS USED IN THE MATCHING OF THE RADIAL WAVE
FUNCTIONS AND THE REGULAR AND IRREGULAR COULOMB WAVE FUNCTIONS
AT THE FITTING RADIUS. THE FORMULA FOR THIS RATIO IS CONTAINED
IN THE APPENDIX OF RAWITSCHERS ARTICLE. THIS CALCULATION REQUIRES
THE RATIO OF THE NORMALIZATION CONSTANTS OF THE POINT COULOMB
RADIAL WAVES. THE FORMULA FOR THE NORMALIZATION CONSTANTS IS
GIVEN IN THE APPENDIX. THE FUNCTION GAM1 USED IN THE VARIABLE
STREAM IS EQUAL TO THE REAL PART OF THE NATURAL LOG OF THE GAMMA
FUNCTION(X+IY), WHERE I IS IMAGINARY I.I.E., SQUARE ROOT OF -1. GAM1
IS FOR CALCULATING VALUES OF GAMMA FUNCTIONS IN THE NORMALIZATION
CONSTANTS RATIO FORMULA.

901 IF((1.+PHIK)-3.)951,953,953
951 XR=(3.141593/2.)*(DABS(SVOFK)-1.-PHIK)-GAM4(PHIK+1.,GM)
GO TO 998
953 XR=(3.141593/2.)*(DABS(SVOFK)-1.-PHIK)-GAM3(PHIK+1.,GM)
998 IF(1.-PHIK)54,55,55
54 IF((PHIK+1.)-3.)957,963,963
957 XI=(3.141593/2.)*(DABS(SVOFK)-1.+PHIK)-(GAM4(PHIK+1.,GM)-DATAN(GM
1/PHIK))
U=DSIN(3.141593*(1.0-PHIK))*CSHY(3.141593*GM)
V=DCOS(3.141593*(1.-PHIK))*SSHY(3.141593*GM)
IF(U)56,57,57
57 ARG=ATAN(V/ABS(U))
GO TO 58
56 ARG=(3.141593-ATAN(ABS(V)/ABS(U)))*V/ABS(V)
58 XI=XI+ARG
GO TO 91
55 IF((1.-PHIK)-3.)59,90,90
59 XI=(3.141593/2.)*(DABS(SVOFK)-1.+PHIK)-GAM4((-PHIK+1.),GM)
GO TO 91
90 XI=(3.141593/2.)*(DABS(SVOFK)-1.+PHIK)-GAM3((-PHIK+1.),GM)
GO TO 91
963 XI=(3.141593/2.)*(DABS(SVOFK)-1.+PHIK)-(GAM3(PHIK+1.,GM)-DATAN(GM
1/PHIK))
U=DSIN(3.141593*(1.0-PHIK))*CSHY(3.141593*GM)
V=DCOS(3.141593*(1.-PHIK))*SSHY(3.141593*GM)
IF(U)751,752,752
751 ARG=(3.141593-ATAN(ABS(V)/ABS(U)))*V/ABS(V)
GO TO 58
752 ARG=ATAN(V/ABS(U))
GO TO 58
91 SRY=-A(8)*((SVOFK*(SVOFK+PHIK)+GP*(GP-GM))/(2.*SQS(SVOFK,GP)))*.

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15 CRY=((SVOFK*(SVOFK-PHIK)+GP*(GP+GM))/(2.*SQS(SVOFK,GP)))*.5
   SRY=A(8)*((SVOFK*(SVOFK-PHIK)+GP*(GP+GM))/(2.*SQS(SVOFK,GP)))*.5
15 CRY=((SVOFK*(SVOFK+PHIK)+GP*(GP+GM))/(2.*SQS(SVOFK,GP)))*.5
   SNKR=SIN(XR)*CRY+SRX+COS(XR)
   CNKR=COS(XR)*CRY-SIN(XR)*SRX
   CNKI=COS(XR)*CRY-SIN(XR)*SRX
   SKRI=-SIN(XR)*CRY-SIN(XR)*SRX
   SKR=SIN(XI)*CRY-SIN(XI)*SRX
   CKRI=COS(XI)*CRY-SIN(XI)*SRX
   CKI=-SIN(XI)*CRY-SIN(XI)*SRX
   TNKP=((SNKR+DCKP*SKR)/(1.+TNKP**2).
   C2NKP=(1.-TNKP**2)/(1.+TNKP**2)
   S2NKP=2.*TNKP/(1.+TNKP**2)
   TNKR=SNKR/CNKR
   CNRP=(1.-TNKR**2)/(1.+TNKR**2)
   SNRP=2.*TNKR/(1.+TNKR**2)
   TNKM=((SNKI+DCKN*SKI)/(1.+TNKM**2)
   C2KM=(1.-TNKM**2)/(1.+TNKM**2)
   TKRM=SNKI/CNKI
   CNRM=(1.-TKRM**2)/(1.+TKRM**2)
   SNRM=2.*TKRM/(1.+TKRM**2)
   TKI=SKI/CKI
   ATA(LOP)=ATAN(TKR)
   ETI(LOP)=ATAN(TKI)
   ETAKP(LOP)=ATAN(TNKR)
   ETAKN(LOP)=ATAN(TKRM)
   ETKP(LOP)=ATAN(TNKP)
   ETKN(LOP)=ATAN(TNKM)

```

ALL OF THE ABOVE STEPS ARE CONCERNED WITH THE CALCULATION OF
6 NEEDED PHASE SHIFTS, SUMMARIZED BELOW:
ATA=IRREGULAR COULOMB PHASE SHIFT FOR SVOFK=+
ETI=IRREGULAR COULOMB PHASE SHIFT FOR SVOFK=-
ETAKP=IRREGULAR COULOMB PHASE SHIFT FOR SVOFK=+
ETAKN=IRREGULAR COULOMB PHASE SHIFT FOR SVOFK=-
ETKP=NUCLEAR PHASE SHIFT FOR SVOFK=+
ETKN=NUCLEAR PHASE SHIFT FOR SVOFK=-
THE MANY STEPS USED ARE BASED ON THE FORMULA FOR THE PHASE SHIFTS
GIVEN IN THE APPENDIX. THE MATHEMATICAL BASIS FOR THE ABOVE STEPS
IS CONTAINED IN THE NOTES HELD BY PROF. BUSKIRK, THE GAM3 AND
GAM4 FUNCTIONS ARE USED IN CALCULATING THE ARGUMENT OF GAMMA FUNC-
TIONS CONTAINED IN APPLICABLE FORMULAS.

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      IF (ABS(ATA(LOP)).LE.(1.0E-50)) ATA(LOP)=0.0
      IF (ABS(ETAKP(LOP)).LE.(1.0E-50)) ETAKP(LOP)=0.0
      IF (ABS(ETAKN(LOP)).LE.(1.0E-50)) ETAKN(LOP)=0.0
      IF (ABS(ETKP(LOP)).LE.(1.0E-50)) ETKP(LOP)=0.0
      IF (ABS(ETKN(LOP)).LE.(1.0E-50)) ETKN(LOP)=0.0
      GO TO JACK,(800,801)
      Q=2,-SNRP*S2NKP-CNRP*C2NKP-S2KM*SNRM-C2KM*CNRM
      TEST=DCKP**2+Q
      IF (TEST-A(14)) 100, 101, 101
CC CC CC CC
      REFERENCE TO DETAILED NOTES WILL VERIFY THAT AS THE VALUE OF TEST
      APPROACHES ZERO THE NUCLEAR PHASE SHIFT APPROACHES THE REGULAR
      COULOMB PHASE SHIFT VALUE.
101 SVFKM=-SVOFK
   SVFK=DABS(SVOFK)+1.000000000000
   LOP=LOP+1
   GO TO 10
CC CC CC CC CC
      IF THE VALUE OF TEST-A(14), WHERE A(14) IS PRESENTLY 0.1D-09, IS
      GREATER THAN ZERO, THEN THE ANGULAR MOMENTUM QUANTUM NUMBER IS
      INCREASED BY 1 AND RETURN TO RECALCULATION OF COULOMB FUNCTIONS
      TAKES PLACE. ALL CALCULATIONS ARE THUS REDONE FOR NEW VALUE OF
      SVOFK.
100 ASSIGN 801 TO JACK
   SVFK=DABS(SVOFK)+1.000000000000
   PHIK=DSQRT(SVOFK**2-ALPHA2)
   IF (LOP-LAG) 905, 905, 105
CC CC CC CC CC CC CC CC
      THE ABOVE STEP TERMINATES CALCULATION OF PHASE SHIFTS WHEN SVOFK
      REACHES VALUE OF LAG. LAG IS SET AT 34 NOW, BUT COULD BE CHANGED
      IF DESIRED. THE VALUE OF LAG DOES NOT AFFECT THE POINT AT WHICH
      NUCLEAR PHASE SHIFTS ARE SET EQUAL TO COULOMB, UNLESS SVOFK VALUE
      EQUAL TO LAG IS REACHED BEFORE TRANSFER TO COULOMB OCCURS. FOR
      INCIDENT ENERGIES LESS THAN 500 MEV, TRANSFER TO COULOMB FUNCTIONS
      WILL OCCUR BEFORE SVOFK=34. FOR HIGH ENERGIES, IT MAY BE DESIRABLE
      TO USE LARGER LAG VALUE TO ENSURE INCLUSION OF ENOUGH VALUES OF
      SVOFK.
905 ETKP(LOP)=ETAKP(LOP)
   ETKN(LOP)=ETAKN(LOP)
   LOP=LOP+1
   GO TO 901
105 CONTINUE
   ETKP(LOP) = ETAKP(LOP)
   ETKN(LOP) = ETAKN(LOP)

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YAL04230
YAL04240
YAL04250
YAL04260
YAL04270
YAL04280
YAL04290
YAL04300
YAL04340
YAL04350
1AY4350
2AY4350
3AY4350
4AY4350
5AY4350
YAL04360
YAL04370
YAL04380
YAL04390
1AY4390
2AY4390
3AY4390
5AY4390
5AY4390
6AY4390
7AY4390
YAL04400
YAL04410
YAL04420
YAL04430
1AY4430
2AY4430
3AY4430
4AY4430
5AY4430
6AY4430
7AY4430
8AY4430
9AY4430
10AY4430
11AY4430
YAL04440
YAL04450
YAL04470
YAL04480
YAL04490
YAL04500
YAL04510

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COR(J,M+1)=COR(K,M)-(SVOFK+1.)*COR(K+1,M)/(2.*SVOFK+3.)-SVOFK*COR(
1K-1,M)/(2.*SVOFK-1.) YAL05000
COI(J,M+1)=COI(K,M)-(SVOFK+1.)*COI(K+1,M)/(2.*SVOFK+3.)-SVOFK*COI(
1K-1,M)/(2.*SVOFK-1.) YAL05010
DOR(J,M+1)=DOR(K,M)-(SVOFK+1.)*DOR(K+1,M)/(2.*SVOFK+3.)-SVOFK*DOR(
1K-1,M)/(2.*SVOFK-1.) YAL05020
DOI(J,M+1)=DOI(K,M)-(SVOFK+1.)*DOI(K+1,M)/(2.*SVOFK+3.)-SVOFK*DOI(
1K-1,M)/(2.*SVOFK-1.) YAL05030
GO TO 128 YAL05040
COR(J,M+1)=COR(K,M)-(SVOFK+1.)*COR(K+1,M)/(2.*SVOFK+3.)) YAL05050
COI(J,M+1)=COI(K,M)-(SVOFK+1.)*COI(K+1,M)/(2.*SVOFK+3.)) YAL05060
DOR(J,M+1)=DOR(K,M)-(SVOFK+1.)*DOR(K+1,M)/(2.*SVOFK+3.)) YAL05070
DOI(J,M+1)=DOI(K,M)-(SVOFK+1.)*DOI(K+1,M)/(2.*SVOFK+3.)) YAL05080
K=K+1 YAL05090
SVOFK=SVOFK+1. YAL05100
IF(M-5)112,135,135 YAL05110
CONTINUE YAL05120
THE ABOVE STEPS CALCULATE THE VALUES OF THE COEFFICIENTS PERTINENT
TO METHOD OF SUMMATION OF LEGENDRE POLYNOMIALS BY REDUCED COEF-
FICIENTS. FOURTH ORDER REDUCED COEFFICIENTS ARE USED IN THIS
METHOD IN THIS PROGRAM. YAL05130
ITHXX = 0 YAL05140
EINCX=EINCX+0.511 YAL05150
A(3)=EINCX YAL05160
I=KMAX-5 YAL05170
ITHXX = ITHXX + 1 YAL05180
THETA=THEXX(ITHXX)/57.29578 YAL05190
SVOFK=0 YAL05200
ZP(1)=1. YAL05210
ZP(2)=COS(THETA) YAL05220
DOI14J=3.1 YAL05230
SVOFK=SVOFK+1. YAL05240
ZP(J)=((2.*SVOFK+1.)*COS(THETA)*ZP(J-1)-SVOFK*ZP(J-2))/((SVOFK+1.)) YAL05250
I=KMAX-5 YAL05260
SVOFK=0 YAL05270
FTH=0 YAL05280
FTI=0 YAL05290
GTH=0 YAL05300
GF=2.*CK*(1.-COS(THETA))**4 YAL05310
DG=DF*SIN(THETA) YAL05320
DOI15K=1.1 YAL05330
FTH=FTH+COR(K,5)*ZP(K) YAL05340
GTH=GTH+DOR(K,5)*ZP(K) YAL05350
YAL05360
YAL05370
YAL05380
YAL05390
YAL05400
YAL05410
YAL05420
YAL05430
YAL05440

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```

C C C
FMOO=(1.0+TP*(RX/CP)**2)*EXP(-(RX/CP)**2)
RETURN
#2 IS A GAUSSIAN P-SHELL CHARGE DISTRIBUTION.
3 C=2.12
C=C*CK
FMOO=EXP(-(RX/C)**2)
RETURN
C C C
#3 IS A GAUSSIAN CHARGE DISTRIBUTION.
4 ALIT=0.0019
BLIT=(4.4)*CK
CLIT=(1.1)*CK
ABIG=(1.649)*CK
BBIG=(1.705)*CK
FMOO=(1.0+(RX/BBIG)**2)*EXP(-(RX/ABIG)**2)+ALIT*EXP(-(RX-BLIT)**2)
CLIT**2)
1 RETURN
C C C C
#4 IS A CARBON-12 CHARGE DISTRIBUTION DEVELOPED FROM WORK AT
STANFORD BUT PRESENTLY CONSIDERED NOT CORRECT.
5 ASMAL=(0.932)*CK
BSMAL=(1.305)*CK
CSMAL2=(0.205)*((CK)**2)
FMOO=(1.0/(8.0*(3.14159)**1.5))*((1.0/ASMAL**3)*EXP(-(RX/(2.0*ASMAL**2))-(4.0*(BSMAL**7))))
1 MAL)**2)-(CSMAL2*(6.0*(BSMAL**2))-(4.0*(BSMAL**7))))
2 *EXP(-(RX/12.0*BSMAL)**2)
RETURN
C C C
#5 IS A LITHIUM-6 CHARGE DISTRIBUTION DEVELOPED BY SUELZLE.
END
YAL05740
YAL05750
1AY5750
2AY5750
3AY5750
YAL05760
YAL05770
YAL05780
YAL05790
1AY5790
2AY5790
3AY5790
YAL05800
YAL05810
YAL05820
YAL05830
YAL05840
YAL05850
YAL05860
1AY5860
2AY5860
3AY5860
4AY5860
YAL05870
YAL05880
YAL05890
YAL05900
YAL05910
YAL05920
YAL05930
1AY5930
2AY5930
3AY5930
YAL05770

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13. ABSTRACT

A phase shift analysis is used to obtain scattering cross sections for incident electrons on Carbon-12 and Lithium-6. Results are given for incident electron energies of 10 - 100 Mev and for scattering angles of 45, 90 and 135 degrees. A gaussian p-shell charge distribution is used for Carbon-12, and an empirical charge distribution developed by L. R. Suelzle is used for Lithium-6. A comparison is also made between the phase-shift results and results obtained using the Born approximation.

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Calculation of electron scattering cross sections for Carbon-Twelve and Lithium-Six using phase shift analysis.

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